Ahmad Ahmad

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Field of Specialization

Field of research is computational modeling and experimental guiding for the growth of multiphase thin films with pillar-in-matrix configurations via physical vapor deposition and chemical vapor deposition using density functional theory, kinetic Monte Carlo method, phase-field method, theory of elasticity, thermodynamics and kinetics, finite element method and Fast Fourier Transform.

Education

1) Purdue University, West Lafayette, IN
PhD in Materials Science and Engineering – Computational Engineering concentration
September 2020 - August 2025
Advisor: Dr. Anter El-Azab

2) Indiana State University, Terre Haute, IN
Bachelor of Science in Chemistry- American Chemical Society Certified Concentration
August 2017 - May 2020
GPA: 3.95/4.0
Bachelor of Science in Physics- Chemical Physics Concentration
August 2017 - May 2020
GPA: 3.95/4.0
Advisor: Dr. Eric Glendening

Research Experience

1) Purdue University, Lafayette, IN
Postdoctoral Associate, department of mechanical engineering December 2025 – Current
Research Assistant, department of materials engineering September 2020 – August 2025

- **"**Mechanical behavior of gradient steel**"** May 2025 – present
  - Utilize a dislocation-based crystal plasticity model to understand recrystallization phenomena in BCC metals.
  - Couple a crystal plasticity finite deformation mechanics model with phase field method to understand the recrystallization phenomena in BCC steel.
- **"**Theoretical modeling of the growth of multiphase thin films with pillar-in-matrix configurations.**"** September 2020 – April 2025
  - Develop highly parallelized kinetic Monte Carlo (kMC) tool to study the growth kinetics in thin films.
  - Develop highly parallelized Fast Fourier Transform (FFT) to solve micromechanics in multiphase systems.
  - Utilize density functional theory (DFT) to parameterize the kMC model for binding and diffusion energy calculations.
  - Develop a highly parallelized coupled FFT-kMC framework that is parameterized using DFT.
  - Understand the effect of surface strains on the diffusion of adatoms and the formation of epitaxial islands in thin films growth using kinetic Monte Carlo compared with nucleation rate theory of submonolayer growth.
  - Generate quantitative data from thermodynamics models to predict the structure morphology of oxide-metal thin films using physics-based machine learning algorithm.
  - Using kinetic rate theory and numerical methods such kMC and phase field to explore scaling laws to identify growth regimes and island nucleation kinetics in multiphase films.
  - Develop framework using interface/surface elasticity theory for curved interfaces and surfaces to correlate interfacial effects on the stresses inside materials (Capillarity forces in solid films).

2) Indiana State University, Terre Haute, IN
Research Assistant, Theoretical study on the ion fragmentation of cyclohexanol September 2019 – May 2020

- Developed a tool to understand the ion-fragmentation in cyclohexanol and energy transfer in mass-spectrometry using density-functional theory and nudged elastic band calculations.

- Used genetic algorithm to understand the different possible configurations of fragmented cyclohexanol at different temperatures using ensemble averaging and correlate with mass-ion spectrum.
- Compared Hartree-Fock method of in-house electronic structure code to compare with DFT results.

Research Assistant, Understanding bond length variation in molecules May 2018 – August 2019

- Use computational chemistry methods with natural bond orbital (NBO) and natural resonance theory (NRT) analyses to explore bond lengths for C-C, C-N, and C-O bonds in amino acids and dipeptides.
- Examined the relationship between bond length, bond order, hybridization, and Coulomb interactions using principal component analysis and multi-linear regression.

Research Assistant, Physical Chemistry January 2018 - May 2018

- "Application of Thermoelectric generators (TEG), Bismuth Telluride, in Undergraduate Experiments"
  - Determine the efficiency as well as the effective thermal conductivity of TEGs using Peltier effect.

Publications

1) Ahmad A. et al, "Effect of elastic strain on growth kinetics of multiphase thin films – A coupled DFT-kMC-FFT approach." To be Submitted to Acta Materialia, August 2025.
2) Ahmad A. et al, "A DFT investigation on the impact of strain on the binding and diffusion energies of adatoms and admolcules on surfaces." To be Submitted to Applied Surface Science, August 2025.
3) Bigdeli, M. A., Ahmad A. et al, "Modeling Growth and Mass Transport Properties of Nanocolumnar Electrodes to Optimize Electrochemical Detection" ACS Applied Engineering Materials, **3,** (2025) 166-1656.
4) Ahmad A. et al, "On the elastic problem of a representative volume element for multiphase thin films." Journal of mechanics and physics of solids, **200**, (2025) 106142.
5) Ahmad A. *et al*, "A DFT-based kinetic Monte Carlo simulations of multiphase oxide-metal thin film growth." Journal of Applied Physics, **135**, (2024) 095307.
6) Rayaprolu S., Ahmad A. *et al*, "Energetic of nanoscale films with self-assembled oxide/metal pillars in nitride matrix." MTLA **30** (2023) 101845.
7) Lu J., …, Ahmad A. *et al*, "Abnormal in-plane epitaxy and formation mechanism of vertically aligned Au nanopillars in self-assembled CeO2-Au metamaterial systems." Materials Horizons, 2023.
8) Starkey K., Ahmad A. *et al*, A generalized 3D elastic model for nanoscale self-assembled oxide-metal thin films with pillar-in-matrix configurations. Acta Materialia, **228** (2022) 117779.

Presentations

1) Ahmad A. and A. El-Azab "DFT-informed kinetic Monte Carlo simulations of multiphase thin films growth." Oral presentation scheduled at USNCCM, July 2025 – Chicago, IN
2) Ahmad A. and A. El-Azab "Elastic strain coupling in DFT-Informed Kinetic Monte Carlo Simulation of Multiphase Thin Film Growth" Oral presentation scheduled at TMS, March 2025 – Las Vegas, NV
3) Ahmad A. and A. El-Azab "Strain Effect on Adatom Diffusion, Island Nucleation and Monolayer Growth on Metal and Oxide Surfaces." Oral presentation scheduled at TMS, March 2025 – Las Vegas, NV
4) Ahmad A. and A. El-Azab "Strain Effect on Adatom Diffusion, Island Nucleation and Monolayer Growth on Metal and Oxide Surfaces." Oral presentation scheduled at MRS, December 2024 – Boston, MA.
5) Ahmad A. "Materials science and engineering at Purdue - DFT-Informed Kinetic Monte Carlo Simulation of Growth of Multiphase Thin Films." Invited departmental seminar talk at Indiana State University, Terre Haute IN – September 2024.
6) Ahmad A. H. Wang and A. El-Azab, "On the elastic problem of a representative volume element for multiphase thin films." (Oral presentation at TMS, March 2024, Orlando FL)
7) Ahmad A. H. Wang and A. El-Azab, "DFT-based Kinetic Monte Carlo Framework for the Growth of Multiphase Thin Films." (Poster presentation at TMS, March 2024, Orlando FL, NanoEx conference, Purdue University – West Lafayette IN, April 2023 and Midwest Nano Day, IUPUI Indianapolis IN, September 2023
8) Starkey K., Ahmad A. *et al*, A generalized 3D elastic model for nanoscale self-assembled oxide-metal thin films with pillar-in-matrix configurations. Oral presentation at MMM October 2022, Baltimore MD)
9) Starkey K., Ahmad A. *et al*, A General Elastic Model for Self-Assembled Metal-oxide Vertical Aligned Nanocomposite (VAN) Thin Films. Oral presentation at TMS March 2022, Online due to Covid)

Teaching Experience

1) Purdue University, West Lafayette, IN

Substitute Lecturer, MSE 508 – Phase transformation in solids August – December 2024

- Substitute course instructor whenever is needed to give lecture. Topics included surface and interface structure in crystalline solids and the methods used to characterize them.

Teaching assistant, MSE 340 – Transport Phenomena January – May 2022

- Conducted office hours to help students with homework and quizzes preparation.
- Substitute course instructor for lecturing purposes whenever needed.

2) Indiana State University, Terre Haute, IN

Chemistry Tutor, Science Help Center January – May 2019

- Helped walk-in students with questions regarding exams, quizzes and homework.

Physical Chemistry & Analytical Chemistry Teaching Assistant Fall 2018, Spring & Fall 2019

- Gave lectures for conducting laboratory experiments.
- Helped students with lab settings and sample preparation.
- Helped students with lab assignments.
- Graded lab assignments, homework and quizzes.

General Chemistry Laboratory, Teaching Assistant. Fall 2018, Spring & Fall 2019

- Gave lectures for conducting laboratory experiments.
- Helped students with lab settings and sample preparation.
- Helped students with lab assignments.
- Graded lab assignments, homework and quizzes.

Math Tutor, Math and Writing Center Fall 2017, Spring 2018

- Helped walk-in students with questions regarding exams, quizzes and homework.

3) Parkland College, Champaign, IL

Science and Math Tutor, Center for Academic Success Spring, Summer, Fall 2016, & Spring 2017

- Helped walk-in students with questions regarding exams, quizzes and homework.

Mentoring students

Ying-Cheng Chen (1st year PhD) Fall 2024 – Summer 2025
Kieran Edmonds (1st year PhD) Fall 2024 – Summer 2025
Mani Manikandan (1st year PhD) Fall 2024

Skills and Abilities

- **Programming**: C/C++, Python, Fortran, OpenMP, MPI, Cuda, PyCuda, OpenCL, PyOpenCL, rocm, Linux OS.
- **Computational software**: VASP, LAMMPS, SPPARKS, Quantum Espresso, MOOSE, Abaqus, PyTorch, Nvidia Modulus, MFEM, FFTW, Gaussian, DFT-FE.
- **AI/ML techniques**: Physics-informed neural networks, graph and convolutional neural networks.
- **Visualization software**: Paraview, Ovito, VESTA, GNU plot, Matplotlib
- **Experimental tools knowledge**: X-ray diffraction measurements, tunneling electron microscope, GC-mass spectrometry, 400 MHz Nuclear Magnetic Resonance, 200 UV/VIS spectrophotometer.
- **Languages**: English, Arabic
- **Certificates**: Fundamentals of accelerated computing with CUDA (Nvidia), Scaling workloads across multiple GPUs with CUDA (Nvidia)

Software Development

1) Ahmad A., SharafEldin K., El-Azab A., MPI-based kinentic Monte Carlo simulations of multiphase thin films growth.
2) Ahmad A., El-Azab A., FFT-based homogenization scheme of heterogeneous structure, (serial and parallel versions).
3) Ahmad A., El-Azab A., Pillar size, density and height analysis using API Ovito Python module.
4) Ahmad A., El-Azab A., Bash and python scripts to calculate binding and activation energies under the influence of elastic strain using VASP.
5) Ahmad, A.; Bennett, M.; Froehlich, A.; Nuyen, C.; Rosenhein, L.; Siner, M.; Glendening, E. TORTILLA Electronic Structure Program – Version 0.2. Department of Chemistry and Physics, Indiana State University, Terre Haute, IN. Based on G. Orsini, *J. Chem. Ed*., 92, 1853-1859 (2015)

Campus and Community Involvement

1) Materials Science and engineering Graduate Student association, Purdue University Fall 2021-Spring 2022

Secretary

- Was in charge of organizing meetings and collecting Meeting Minutes information.

2) Purdue Volunteering events Fall 2022 - Spring 2023

- Purdue Space Day (Fall 2022) – helped with monitoring students and completing their working tasks.
- Purdue Math day for the state of Indiana (Spring 2023), helped with grading students' exams.

2) Society of Physics Students members Chapter, Indiana State University August - December 2019

Vice president

- Held tutoring help sessions for freshman and sophomore level physics courses.

2) American Chemical Society members Chapter, Indiana State University September 2018 - September 2019

Active member

- Volunteered in any events that are held by the chapter like chemistry and physics demonstration for kids.

3) Timmy Global Health chapter, Indiana State University November 2018 - May 2019

Active member

- Volunteer at Tucker's House in Nashville, TN during Fall break, and other fundraising events.

4) Muscular Dystrophy Association, Central Illinois chapter

Camp Counselor, Normal, IL July 2017

- Volunteered with 130 service hours for MDA summer camp in July, 2017 to work with children with disabilities.

6) Carle Hospital, Urbana, IL

Student Volunteer in the cardiovascular wing department January – May 2017

- Helped Carle nurses with transporting patients and answering emergency calls from patients as needed.

Professional Membership

1) The minerals, metals and materials society (TMS), student member January 2022 - present

2) Materials research society (MRS), student member August 2024 – present

3) Sigma Pi Sigma, Lifetime Honrary member May 2022 – Present

4) American Chemical Society (ACS), Honorary member January 2020 – May 2023

5) American Physics (APS), Student member May 2020 – May 2021

6*) Society of Physics students (SPS),* Student member May 2018 – May 2020

Peer Reviewer

1) The journal of Applied Physics January 2024 - present

2) Review of Scientific instruments online January 2024 - present

3) Materials and simulation in materials science and engineering August 2024 - present

Relevant courses

Phase transformation in solids, thermodynamics and kinetics in materials, statistical mechanics, defects in solids, computational methods in interfacial phenomena, quantum mechanics, computational methods in materials science, classical mechanics, continuum mechanics, theory of elasticity, introduction to parallel programming, physical chemistry, math methods in physics.

Academic Awards and Scholarships

1) Indiana State University, Terre Haute, IN

- Dean's List all semesters at ISU
- William H. Bell Award in Chemistry May 2019
- Physics Foundation Scholarship May 2019
- Frank L. Miklozek Memorial Scholarship May 2019
- D.J. Reuland Scholarship in Chemistry May 2018
- P.D. Wilkinson Scholarship in Chemistry May 2018
- National American Chemical Society Undergraduate Award in Physical Chemistry March 2018

- International Merit-based Scholar Award August 2017

2) Parkland College, Champaign, IL

- Dean's List all semesters at Parkland
- Honors Scholarship May 2017